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Short Communication

A modified simulated annealing algorithm for estimating solute transport parameters in streams from tracer experiment data

J.Q. Guo[a], L. Zheng[b,*]

[a]Department of Water Resources Engineering, Chang An University, Xi'an, Shanxi, PR China
[b]Centre for Agricultural Resources Research, IGDB, Chinese Academy of Sciences, Shijiazhuang, Hebei, PR China

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Abstract

It is difficult to estimate solute transport parameters in streams empirically and numerous approaches have been investigated in the past. In the current study, we explored the use of the simulated annealing (SA) algorithm for estimating solute transport parameters in streams from tracer experiment data. For a simple one-dimensional dispersion test case, the standard SA algorithm was very slow to converge. To remedy the problem of slow convergence of the annealing optimization, we proposed three strategies to modify the standard SA algorithm and improve the converging speed. The proposed three strategies are: (1) imposing parameter space constraints; (2) adding a valve value for inner loop break; and (3) including an inner loop memory function. We conducted a numerical experiment to test and demonstrate the effectiveness of the modified SA algorithm for estimating three major solute transport parameters: longitudinal dispersion coefficient, cross-sectional averaged flow velocity, and tracer mass loading. We then discussed the advantages and limitations of the proposed algorithm.

Keywords: Solute transport in stream; Simulated annealing; Dispersion coefficient; Parameter estimation

Software availability

Name of Software:	SAST
Developers:	Jian-Qing Guo and Li Zheng
Contact address:	Department of Water Resources Engineering, Chang An University, Xi'an, Shanxi, P. R. China
Telephone:	+86 311 588 5030
Fax:	+86 311 587 1620
E-mail address:	guojian0248@sohu.com
Availability:	freely available by e-mailing your request to guojian0248@sohu.com or zhengli_usa@yahoo.com

1. Introduction

Important parameters that govern the transport of solute in streams include longitudinal dispersion coefficient D_L, cross-sectional averaged velocity v etc. The most common way for determining these parameters is through conducting tracer experiments and analysing the observed tracer concentration profiles. Methods for estimating transport parameters from tracer data were mostly based on approximating Taylor's analytical solution (1954), and often plagued by the errors introduced by the approximation and numerical integration etc. Singh and Beck (2003) gave a detailed account on the limitations of these methods, and proposed a new routing method that is free from the previously mentioned errors. They then applied Marquardt Method to solve the nonlinear least square problem to obtain optimal parameter estimates. In a separate report, Singh (2003) proposed a new method for the treatment of stagnant zones in

* Corresponding author. Tel./fax: +86 311 587 1620.
E-mail address: zhengli_usa@yahoo.com (L. Zheng).

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streams and also applied similar non-linear regression approach to estimate optimal solute transport parameters. Other recent works on estimating solute transport parameters in streams include Swamee et al. (2000), Deng et al. (2002) and Seo and Baek (2004). Detailed surveys of historical development of this line of research can be found in these works.

When analytical expressions for concentration profiles are available, gradient search based non-linear regression algorithms such as Marquardt Method are commonly used to obtain optimal transport parameter estimates. The applications of these methods, however, require the objective function to be smooth, which may not always be the case for complex objective functions. Further, for the applications where local optimal solutions existed, non-unique solutions could result from different initial parameter values (Li et al., 1999). In the current study, we explored the possibility of using a non-gradient based direct search algorithm, the simulated annealing (SA), for optimal solute transport parameter estimation. Such an exploration to our knowledge has not been attempted before.

Simulated annealing (SA) is a global optimization technique that is not based on gradient search. Instead it was derived from statistical mechanics by mimicking the physical annealing process (i.e., the cooling of molten substances to crystalline lattices of minimum energy). Kirkpatrick et al. (1983) first proposed and demonstrated the use of SA in solving the combinatorial optimization problems. The application of SA was later extended to the optimization of continuous functions (e.g., Bohachevsky et al., 1986). Recently, SA also found applications in problems of groundwater management (e.g., Johnson and Rogers, 2001), agricultural water management (e.g., Kuo et al., 2001), and parameter estimation for solute transport in porous media (Li et al., 1999). In this paper we explored the use of SA for estimating solute transport parameters in streams from tracer experiment data. For a simple one-dimensional transport problem, we found that the standard SA algorithm was very slow to converge. To speedup the SA optimization, we proposed three strategies to modify the standard SA algorithm, including (1) imposing parameter space constraints; (2) adding a valve value for inner loop break; and (3) including an inner loop memory function. We then used a numerical experiment to test and demonstrate the effectiveness of the modified SA algorithm for estimating solute transport parameters in streams.

2. Simulated annealing and its improvement

2.1. Standard simulated annealing algorithm

Inspired by the Monte Carlo method introduced by Metropolis et al. (1953), Kirkpatrick et al. (1983) developed the SA technique for the optimization of combinatorial problem. It makes the analogy between the state of each molecule that determines the energy function and the value of each parameter that affects the objective functions. It then uses the statistical mechanics principle for energy minimization to minimize the objective function and optimize the parameter estimates. Starting with a high temperature, it randomly perturbs the parameter values and calculates the resulting objective function. The new state of objective function after perturbation is then accepted by a probability determined by the Metropolis criterion. The system temperature is then gradually reduced as the random perturbation proceeds, until the objective function reaches its global or nearly global minimum (Kirkpatrick et al., 1983). A typical SA algorithm is described as follows (also see Fig. 1):

Step 1 Specify initial temperature $T_k = T_0$ for $k = 0$; randomly initialize the parameter set estimate $\theta^* = \theta_0$.

Step 2 Under kth temperature, if the inner loop break condition is met, go to step 3; otherwise, for $(j+1)$th perturbation, randomly produce a new parameter set θ_{j+1}, compute the change in objective function $\Delta f = f(\theta^*) - f(\theta_{j+1})$. If $\Delta f \leq 0$, accept $\theta_{j+1}(\theta^* = \theta_j)$; if not, follow the Metropolis criterion to accept θ_{j+1} with a probability of $\min\left(1, e^{-\Delta f/T_k}\right)$ and step 2 continues.

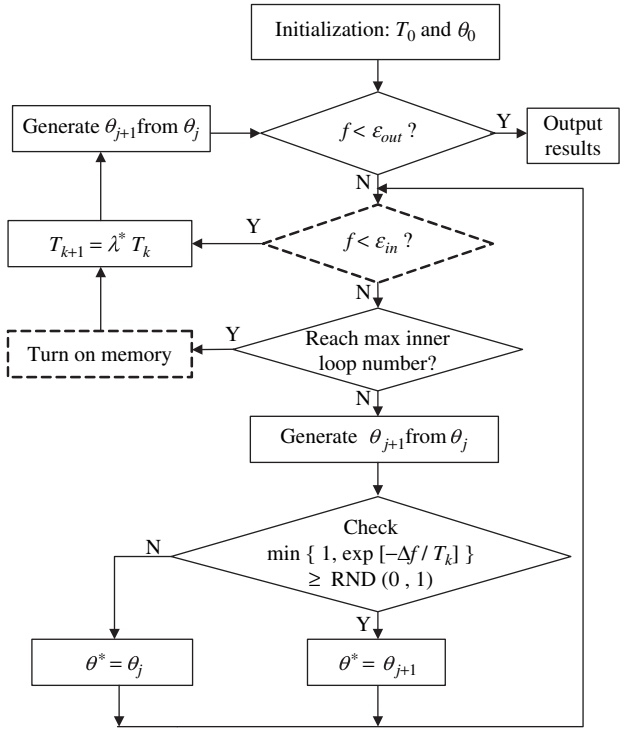

Fig. 1. The flow chart of modified SA algorithm. Boxes with solid lines are original SA algorithm components, and boxes with dashed lines are added new components.

Step 3 Reduce T_k to T_{k+1} following a specified cooling schedule. If outer loop break condition is met, computation stops and optimal parameter set is reached; if not, return back to step 2.

The steps outlined above consist of one inner loop (step 2) and one outer loop (step 3). The proceeding of SA is mainly controlled by (1) the choice of T_0; (2) the way a new perturbation is generated; (3) the inner loop break conditions; (4) the choice of cooling schedule; and (5) the outer loop break conditions. We will specify these control conditions later in our SA implementation.

2.2. Modified simulated annealing algorithm

The slow convergence of standard SA algorithm is a common drawback in its application. As demonstrated in the application given later, a similar problem existed in using standard SA for a simple one-dimensional dispersion problem. It is therefore necessary to modify the standard SA algorithm to speedup the convergence and reduce the computational cost. In this study we proposed following three strategies to improve the SA optimization speed:

(1) *Parameter space constraints*: theoretically any non-negative real numbers could be the transport parameter values. In a specific application, however, practitioners can often specify a much narrower range for each parameter to be estimated. Obviously, the narrower the range is, the faster it will be for the computation to converge.
(2) *A valve value for inner loop break*: normally a maximum number of perturbations within each temperature (or the so called Markov chain length) is specified as the inner loop break condition. In addition to that, we specified an inner loop valve value ε_{in} to break the inner loop iteration when $f < \varepsilon_{in}$.
(3) *Inner loop memory*: normally the end of inner loop parameter estimates will be passed onto the next loop after the temperature is reduced. We added a memory function to the inner loop which would remember the parameter set of the minimum objective function occurred during current inner loop, and used it as the beginning parameter estimates for the next inner loop.

Fig. 1 gives a flow chart of the modified SA algorithm as explained above.

2.3. Objective function and simulation control conditions

To determine the solute transport parameters, such as the longitudinal dispersion coefficient D_L and cross-sectional averaged flow velocity v, from trace tests, we used Taylor's (1954) analytical solution for concentration variation along the stream length after an instantaneous release of certain tracer mass. The solution can be written as:

$$c(x,t) = \frac{M}{A\sqrt{4D_L\pi t}} \exp\left(-\frac{(x-vt)^2}{4D_L t}\right) \tag{1}$$

where c – the tracer concentration; M – the mass of tracer released at $x = 0$ and $t = 0$; A – the cross-sectional area of the stream; t – time; x – the distance between the sampling spot and tracer released point.

To apply SA optimization for parameter estimation, we define the objective function f as

$$f(\theta^*) = \frac{1}{n}\sum_{i=1}^{n}\left(c_i^o - c_i^c\right)^2 \tag{2}$$

where θ^* – the parameter set estimate; c_i^o – the ith observed tracer concentration; c_i^c – the corresponding ith tracer concentration computed by using Eq. (1) and θ^*; n – the number of observations. The goal of SA optimization is to find a set of θ^* that will minimize f as defined in Eq. (2). In our exercise, we used (D_L, v, m) as the unknown parameter set to be estimated, where m is the tracer mass loading intensity and is defined as M/A.

To implement the modified SA, we specified the simulation control conditions as follows.

(1) *Initial temperature*: we determined the initial temperature using the following formulae:

$$\chi_0 = \exp\left(\frac{-\bar{\Delta}f^+}{T_0}\right) \tag{3}$$

where χ_0 is the initial probability for acceptance, and was set as 0.8 in current work; $\bar{\Delta}f^+$ is the averaged increment of objective function over the averaged value of objective function after multiple perturbations. Here we used 10 000 times of perturbations to determine $\bar{\Delta}f^+$ and calculate T_0.
(2) *Perturbation generating function*: we used uniform random number to produce parameter set perturbation. The new parameter set $\theta_{j+1} = \theta_j + \rho\theta_j\,[0.5 - \mathrm{RND}(0,1)]$, where θ_j is the current parameter set estimate; θ_{j+1} is the parameter set after perturbation; ρ is the perturbation coefficient, $=0.1$ in current study; RND(0,1) is an uniform random number between 0 and 1.
(3) *Cooling schedule*: we used a power cooling schedule for temperature reduction, which is $T_{k+1} = \lambda T_k$ with $0 < \lambda < 1$. We varied λ between 0.4 and 0.95 in the current study.

(4) *Inner loop break conditions*: the inner loop will break when the number of iteration exceeds the specified Markov chain length or when $f < \varepsilon_{in}$. We varied ε_{in} between 0.005 and 0.00005 in the current study.
(5) *Outer loop break conditions*: the outer loop will break when the number of outer loop exceeds 12 000 or when $f < \varepsilon_{out}$, the outer loop valve value which was specified as 0.00005 in the current exercise. If the outer loop breaks before f reaches ε_{out}, we consider that the SA optimization failed to converge.

3. Numerical tests and results

We assumed an ideal transport of certain tracer mass after an instantaneous release in a one-dimensional stream. Further we assumed no measurement errors. We then used Eq. (1) and a set of true parameters ($D_L = 3000\ m^2/min$; $v = 30\ m/min$; $m = 0.5\ kg/m^2$) to generate a series of (c_i^o, t_i) at $x = 500$ m as given in Table 1.

We assumed D_L, v, and m values were unknown and to be estimated, and specified their possible ranges as $300 < D_L < 30\,000$, $3 < v < 300$, and $0.05 < m < 5.0$. We then applied the modified SA algorithm and control conditions given above to the observed data series in Table 1 and obtained the best estimates of the transport parameters as $D_L = 3052.8\ m^2/min$; $v = 29.8\ m/min$; $m = 0.504\ kg/m^2$, all were within 3% relative error margin compared to the true values given before.

When the standard SA algorithm was used, the outer loop iteration number exceeded 12 000, the maximum outer loop number specified, regardless of the choice of Markov chain length. The use of three strategies mentioned before would dramatically speedup the rate of convergence. Table 2 lists the numbers of outer loop iteration needed for convergence corresponding to the various choices of Markov chain length and ε_{in} values. In these cases λ was set at 0.90. Table 3 gives the outer loop iteration numbers needed for various Markov chain length and λ values. In these cases ε_{in} was set at 0.00005.

From Tables 2 and 3 it is obvious that the modification to the standard SA algorithm has dramatically improved the optimization speed. The choice of Markov chain length seems to have limited impacts on the computational speed. The choice of ε_{in} value, however, has a major impact. When ε_{in} is approaching ε_{out}, the impacts become most significant. The value of λ is also a significant factor in determining the converging speed. Our numerical experiments indicated that the best choice of λ value is between 0.4 and 0.65.

Table 1
Observed concentration time series at $x = 500$ m

t_i (min)	6	10	12	14	16	20	24	36
c_i (mg/l)	0.254	0.583	0.649	0.663	0.642	0.552	0.444	0.197

Table 2
The outer loop iteration numbers and the corresponding Markov chain length and ε_{in} values

Cooling rates λ	The lengths of Markov chain					
	100	300	500	800	1200	1600
0.95	123	170	208	195	267	147
0.90	110	121	82	128	81	85
0.85	104	90	84	107	57	62
0.80	103	109	80	90	56	75
0.75	47	55	64	46	117	87
0.70	87	43	141	80	56	56
0.65	50	144	27	65	36	22
0.60	27	47	34	20	53	40
0.50	59	23	34	21	24	59
0.40	42	64	21	25	37	33

4. Discussions and conclusions

From the above tests and analyses, we conclude that the modified SA algorithm provides an effective and speedy optimization technique for the specific parameter estimation problem we defined in this study. For this initial assessment of SA algorithm, we limited our applications to an ideal one-dimensional transport problem in order to simplify the analyses. For field application, however, we need to further assess the proposed algorithm with more realistic cases, i.e. non-uniform velocity distribution and dead zones, pockets of low velocity, natural meandering streams etc. Concentration solutions given in Singh (2003) and Swamee et al. (2000) for example will provide good starting points for such further assessments. The performance of SA in these more realistic transport cases can then be examined against empirical and theoretical methods proposed by other authors (e.g., Deng et al., 2002; Seo and Baek, 2004).

The use of additional constraints to speed up the SA convergence is not without its danger. The more constraints we impose (e.g., the use of inner loop memory function), the faster the computation will converge, however, the less freedom the random perturbation will have, and thus the more danger of getting trapped in local minima. Fortunately, for the parameter estimation problem we study, we know by a priori that the theoretical global minimum of the objective function is zero, i.e. the predicted concentrations would perfectly match the observations. As long as we specify an outer loop valve value close enough to zero, the parameter estimates obtained by a converged SA optimization should be at least near global minimum.

Table 3
The outer loop iteration numbers and the corresponding Markov chain length and λ values

Inner valve values	The lengths of Markov chain							
	100	300	500	800	1200	1600	2000	3000
0.05	10 390	4356	6103	970	6735	5029	4023	4957
0.01	955	692	700	222	121	253	488	280
0.0075	150	261	282	204	217	150	221	165
0.005	163	107	133	255	115	587	120	206
0.001	134	105	106	122	81	126	82	172
0.00075	127	121	82	155	81	112	100	82
0.0005	110	121	82	128	81	85	126	84

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